



**University of
Zurich**^{UZH}

**Zurich Open Repository and
Archive**

University of Zurich
University Library
Strickhofstrasse 39
CH-8057 Zurich
www.zora.uzh.ch

Year: 2012

Acta Crystallographica Section C in 2012

Linden, Anthony

DOI: <https://doi.org/10.1107/S0108270111054916>

Posted at the Zurich Open Repository and Archive, University of Zurich

ZORA URL: <https://doi.org/10.5167/uzh-53891>

Journal Article

Published Version

Originally published at:

Linden, Anthony (2012). Acta Crystallographica Section C in 2012. Acta Crystallographica. Section C, Crystal Structure Communications, 68(1):e1-e2.

DOI: <https://doi.org/10.1107/S0108270111054916>

Acta Crystallographica Section C in 2012

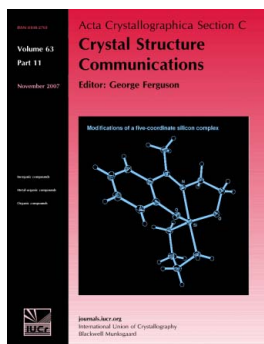
Anthony Linden

Acta Cryst. (2012). **C68**, e1–e2

Copyright © International Union of Crystallography

Author(s) of this paper may load this reprint on their own web site or institutional repository provided that this cover page is retained. Republication of this article or its storage in electronic databases other than as specified above is not permitted without prior permission in writing from the IUCr.

For further information see <http://journals.iucr.org/services/authorrights.html>



Acta Crystallographica Section C: Crystal Structure Communications specializes in the rapid dissemination of high-quality studies of crystal and molecular structures of interest in fields such as chemistry, biochemistry, mineralogy, pharmacology, physics and materials science. The numerical and text descriptions of each structure are submitted to the journal electronically as a Crystallographic Information File (CIF) and are checked and typeset automatically prior to peer review. The journal is well known for its high standards of structural reliability and presentation. *Section C* publishes approximately 1000 structures per year; readers have access to an archive that includes high-quality structural data for over 10000 compounds.

Crystallography Journals **Online** is available from journals.iucr.org

Acta Crystallographica Section C in 2012

Anthony Linden

Institute of Organic Chemistry, University
of Zurich, Winterthurerstrasse 190,
CH-8057 Zürich, Switzerland
E-mail: alinden@oci.uzh.ch

Acta Crystallographica Section C was pleased to be able to publish its first virtual special issue at the beginning of December, 2011. The issue focussed on polymorphism (http://journals.iucr.org/special_issues/2011/polymorphism/), was highlighted on the IUCr homepage and has received favourable comment. We are therefore encouraged to proceed with plans for the next special issue to be published towards the end of 2012. The issue will focus on **absolute structure**.

The unambiguous determination of absolute structure, particularly where the absolute configuration of an enantiomerically pure chiral molecule is needed, is important not only for synthetic and natural product chemists, who wish to fully characterize their products, but can be a critical step for the pharmaceutical industry, where opposite enantiomers of a drug can have quite different biological properties. One of the remaining difficulties since the introduction of the 'Flack parameter' (Flack, 1983) has been a reliable absolute structure determination for materials containing only light atoms (e.g. C, H, N, O) when no other chemical or physical knowledge about the chirality of a substance is available. However, there have been recent advances in methods for evaluating the contribution of resonant scattering to reflection intensities (the Friedel differences), while the advent of dual radiation CCD diffractometers means that more laboratories once again have routine access to Cu $K\alpha$ radiation, thereby allowing more successful absolute structure determinations to be carried out for light-atom structures. Therefore, the results of crystal structure determinations which demonstrate new successes and remaining limitations in the field of absolute structure determination are of particular interest.

The next virtual special issue will include papers in which an absolute structure determination (successful or unsuccessful) is reported. Papers that have been accepted for publication between January, 2011 and September 30, 2012 will be included. Authors interested in contributing new papers for this virtual issue only need to submit their papers to *Section C* in the usual way in the coming months. These will be published shortly after they are accepted, as normal, and then collated into the virtual issue towards the end of the year. Authors do not need to make any special request to have their paper included.

It is pleasing to see more papers containing an extensive discussion of the presented structures along with detailed comparisons with related structures or a discussion of the properties of the material derived from other analyses [for example, Pérez *et al.* (2012), Bekö *et al.* (2012) and Pourayoubi *et al.* (2011)]. Authors are encouraged to submit papers of this kind.

We were saddened to learn of the sudden death of one of our Co-editors, Andrés Goeta, in July 2011. Andrés was not only an excellent Co-editor, but was a highly valued member of the crystallographic community at the University of Durham, UK, and in the UK in general. He came to Durham from Argentina as a post-doctoral fellow in 1995 and then, from 1998, was the X-ray Service Manager for the chemistry department. He was one of the lecturers, and more recently the organizer, of the biannual BCA/CCG Intensive Teaching School in X-ray Structure Analysis. He was also a member of the British Crystallographic Association Council. A most appropriate obituary written by Professor Judith Howard can be viewed at http://www.dur.ac.uk/crystallography.group/Andres_Goeta.html. Andrés will be sadly missed by everyone.

Several *Section C* Co-editors retired at the IUCr Congress last August and it is my pleasure to record here my sincere appreciation of their sustained outstanding efforts and their support of the journal. Some of them have been active Co-editors for a long period, with the longest serving having been involved for about 17 years. The retirees are Jean-

Claude Daran, Graeme Gainsford, Christopher Glidewell, Peter Jones, Phil Squattrito, Helen Stoeckli-Evans (now a Section Editor for *Acta Crystallographica Section E*) and Karl Törnroos. Warm thanks also go out to all current *Section C* Co-editors (listed on the inside front cover) and the Chester Editorial Office staff for their dedicated support and contributions to the ongoing daily operations of the journal.

References

- Bekö, S. L., Thoms, S. D., Schmidt, M. U. & Bolte, M. (2012). *Acta Cryst.* **C68**, o28–o32.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Pérez, H., Corrêa, R. S., Plutín, A. M., O'Reilly, B. & Andrade, M. B. (2012). *Acta Cryst.* **C68**, o19–o22.
- Pourayoubi, M., Tarahhomi, A., Saneei, A., Rheingold, A. L. & Golen, J. A. (2011). *Acta Cryst.* **C67**, o265–o272.